

## REPORT DOCUMENTATION PAGE

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Fifth Conference on Molecular Reaction Dynamics in Condensed  
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F49620-98-1-0181

6. AUTHORS

Dana D. Dlott

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)  
Board of Trustees, University of Illinois at Urbana Champaign

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Approved for public release;  
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13. ABSTRACT (Maximum 200 words)

The Fifth Conference on Molecular Reaction Dynamics in Condensed Matter was held Feb. 10-13 at Newport Beach California, sponsored by AFOSR and ONR, and organized by D. Dlott and A. Apkarian. (Apkarian took over from Charles Wight of Utah). There were 42 attendees, including professors, graduate students, postdoctoral fellows, and technical staff members from national laboratories (LANL, PNL, NIH, etc.). 34 talks were presented. There were 21 invited talks (50 minutes with discussion) and 13 contributed talks (20 minutes with discussion). Lively discussion went on late into the morning.

Symposia on the following topics were presented:

1. Nanochemistry
2. Condensed phase dynamics and chemical reactions
3. Vibrational relaxation

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## 1. Cover sheet for Final Progress Report to AFOSR

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Contract/Grant No. F49620-98-1-0181

Title of project: Fifth Conference on Molecular Reaction Dynamics in Condensed Matter

Reporting period: 01 Jan. 1998 -- 31 May 1998

## 2. Status of effort

The Fifth Conference on Molecular Reaction Dynamics in Condensed Matter was held Feb. 10-13 at Newport Beach California, sponsored by AFOSR and ONR, and organized by D. Dlott and A. Apkarian. (Apkarian took over from Charles Wight of Utah). There were 42 attendees, including professors, graduate students, postdoctoral fellows, and technical staff members from national laboratories (LANL, PNL, NIH, etc.). 34 talks were presented. There were 21 invited talks (50 minutes with discussion) and 13 contributed talks (20 minutes with discussion). Lively discussion went on late into the morning.

Funding provided by AFOSR and ONR was used to reimburse travel and lodging for invited speakers. Vouchers for all available funding have been submitted and it is expected that all available funds will be used when these vouchers have finally cleared.

Symposia on the following topics were presented:

4. Nanochemistry
5. Condensed phase dynamics and chemical reactions
6. Vibrational relaxation

A list of attendees and a summary of talks presented is attached.

# FIFTH SYMPOSIUM ON MOLECULAR REACTION DYNAMICS IN CONDENSED MATTER

Newport Beach, CA

Program Chairs: D. Dlott (Illinois) and A. Apkarian (Irvine)

Program sponsors: Air Force Office of Scientific Research, Office of Naval Research

**Wednesday, Feb. 10**

Arrival and check in

6:00 - 8:00 pm Reception

8:00 - 10:00 pm *Nanochemistry I*-- chair TBA

8:00	Benny Gerber	Irvine	Photodissociation, Electronic Relaxation and Recombination in Molecular Clusters and Solids
8:50	Alex Bendirskii	Irvine	Solvation and dissipation dynamics in a quantum solvent (Hell)
9:10	Mostafa A. El-Sayed	Georgia Tech	Interesting Properties of Matter Confined in Space and Time

**Thursday, Feb. 11**

7:30 - 9:00 am Breakfast

9:00 -12:00 noon *Condensed phase dynamics I* - Chair TBA

9:00	David Tannor	Weizman	Phase Space Approach to Quantum Condensed Phase Dynamics.
9:50	Ben Schwartz	UCLA	Non-linear Non-Polar Solvation Dynamics in Water.
10:10	Bern Kohler	Ohio State	Ultrafast photoionization dynamics of biologically significant molecules in polar solvents
10:30	Break		
10:50	Roseanne Sension	Michigan	Time-resolved studies of conformational relaxation and energy redistribution in simple photochemical reactions
11:40	Todd Martinez	Illinois	<i>Ab Initio</i> Quantum Dynamics of Photoinduced cis-trans Isomerization

12:00 -2:00 pm

Lunch

2:00 -6:00 pm

*Vibrational Relaxation I* --chair TBA

2:00	Alfred Laubereau	TU-Munich	Structure and Hydrogen Bond Dynamics of Water from Subpicosecond Holeburning Spectra in the Infrared
2:50	Mark Berg	South Carolina	Inertial and Diffusive Dynamics in Electronic, Rotational and Vibrational Relaxation
3:40	Break		
4:00	Dana Dlott	Illinois	Ultrafast vibrational energy transfer in liquids
4:50	David Jonas	Colorado	Solvent reorganization dynamics and electronic dephasing in two-dimensional electronic spectra
5:10	Richard Stratt	Brown	How liquids are anharmonic

6:00 - 8:00 pm

Dinner

8:00 - 10:00 pm

*Condensed Phase Dynamics II*--Chair TBA

8:00	Charles Harris	Berkeley	Femtosecond Infrared Studies of Bond Activation Reactions
8:50	Jeff Cina	Oregon	Pulse-shape effects in electronically resonant ultrafast spectroscopy
9:10	Bruce Berne	Columbia	No title

Friday, Feb. 12

7:30 - 9:00 am

Breakfast

9:00 -12:00 noon

*Condensed Phase Dynamics III*--chair TBA

9:00	Robert Silbey	MIT	Fluctuations in low temperature glasses and their effect on spectroscopic measurements (Photon echoes, hole burning and single molecule spectroscopy)
9:50	Michael Ovchinnikov	Irvine	Accurate, non-additive many-body potentials: hydrogen bonding
10:10	Steve Bradforth	USC	Ultrafast studies of electron photodetachment in solution
10:30	Break		

10:50	Michael Fayer	Stanford	Dynamics in Liquids and Glasses Studied with Vibrational Echo Experiments
11:40	Craig Tarver	Livermore	Non-equilibrium processes during shock initiation and deflagration-to-detonation transition in solid explosives

12:00 -2:00 pm

Lunch

2:00 -6:00 pm

*Nanochemistry I*-- chair TBA

2:00	William Eaton	NIH	Kinetics and Dynamics of Elementary Processes in Protein Folding
2:50	Mark Johnson	Yale	Vibrationally mediated electron relaxation in negatively charged water?
3:40	Break		
4:00	Sunney Xie	PNNL	Chemical Dynamics of Single Enzyme Molecules
4:50	Doug Tobias	Irvine	Molecular Dynamics Simulation of Glassy Behavior in Proteins
5:10	Carl Lineberger	Colorado	"Solvent-mediated spin-orbit relaxation in size selected cluster ions"

6:00 - 8:00 pm

Dinner

8:00 - 10:00 pm

*Vibrational relaxation II* -- Chair TBA

8:00	James Skinner	Wisconsin	Solvation dynamics and vibrational relaxation in liquids and supercritical fluids
8:50	Grant Goodyear	Davis	Inhomogeneous vibrational dynamics in compressible supercritical fluids
9:10	Jürgen Troe	Gottingen	Quantitative characterization of the deactivation of highly vibrationally excited molecules in condensed phases.

Saturday, Feb. 13

7:30 - 9:00 am

Breakfast

9:00 - 12:30

*Condensed Phase Dynamics IV*--chair TBA

9:00	Ken Janda	Irvine	Charge Migration and Energy Accomodation in Liquid Helium Nano-Clusters
9:50	Dave Moore	Los Alamos	Time- and space-resolved optical probing of the shock risetime in thin aluminium films
10:10	Jianshu Cao	MIT	Spectral analysis of electron transfer kinetics
10:30	Break		
10:50	Casey Hynes	Colorado	Proton Transfer Reactions at the Ice Surface in Connection with Stratospheric Ozone Depletion
11:40	Craig Martens	Irvine	Simulation of coherent ultrafast processes in condensed phase systems

12:30

*Conference ends*

5th International Conference on Molecular Reaction Dynamics in Condensed Matter  
Hyatt Newporter, Newport Beach, CA  
February 10 - 13, 1999

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